

Brownian One-Body Dynamics in Nuclei

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A novel method is presented for introducing fluctuations in one-body dynamics. It consists of employing a Brownian force in the kinetic equations. For nuclear matter within the spinodal zone, the magnitude of the Brownian force can be determined by demanding correspondence with the growth of the most unstable mode, as given by Boltzmann-Langevin simulations. The method is illustrated and tested for idealized two-dimensional matter and promises to provide a practical means for addressing catastrophic nuclear processes.

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Transport phenomena occur in many physical systems. The approach pioneered by Boltzmann has proven particularly useful and has provided a good understanding of gas kinetics in various fields. For interacting gases, for example, of van der Waals type, the interparticle forces can be taken into account by a mean field. In particular, the nuclear Boltzmann equation [Boltzmann-Uehling-Uhlenbeck (BUU)] forms a very successful framework for understanding a variety of features associated with nuclear collisions at intermediate energies, including collective flow and particle production [1,2].

In the standard Boltzmann treatment, only the average effect of the collisions between the particles of the considered system is included. This leads to a deterministic description and single dynamical trajectory results. While this simplification may be well suited in many physical situations in which the dynamics appears to be rather stable, it cannot provide a description of processes involving instabilities, bifurcations, or chaos. For example, in nuclear physics the BUU approximation is appropriate during the early stages of a nuclear collision, when the system is hot and compressed, but it becomes inadequate if instabilities occur, such as when expansion and cooling has brought the bulk of the system within the spinodal zone of the phase diagram. In such scenarios, it is essential to include the fluctuations as well.

In many branches of physics such diffusive behavior is described by transport theories originally developed for Brownian motion. These approaches simulate the effects of the unretained degrees of freedom by a random term in the dynamics of the retained variables. This idea has inspired an extension of the Boltzmann approach which considers the collisions as random processes so that the fluctuating collision term acts as a Langevin stochastic term on the one-body density [3]. Accordingly, this approach has been denoted the Boltzmann-Langevin (BL) model.

A numerical simulation method was subsequently developed on a phase-space lattice [4,5]. This method has been shown to exhibit the correct relaxation properties

[5–7] and also to describe the spontaneous agitation and propagation of collective modes in unstable nuclear matter [8,9]. Thus, the lattice simulation method provides a well-founded means for solving the BL equation in a numerically reliable manner.

However, the application of this method to realistic scenarios is a formidable task, due to the effort associated with the detailed simulation of all the possible elementary two-body scattering processes on the lattice. A significant advance was made recently by the derivation of simple approximate expressions for the BL transport coefficients at equilibrium, reducing the required numerical effort by several orders of magnitude [10]. Even so, the lattice simulation of the BL transport problem is still too tedious to provide a very useful practical tool for the understanding of physical processes. Therefore, it is worthwhile exploring ways of further simplifying the treatment so that realistic calculations can be made with relative ease, thereby facilitating the confrontation between theory and experiment.

In this Letter, we present a novel method that appears to bring this goal within reach. It consists of replacing the actual complicated (hence computer demanding) fluctuating part of the collision term δI by the effect of an externally imposed Brownian force δF that is suitably tuned so that the dynamics of certain important collective modes is in good accordance with the results of the complete BL model. Specifically, since we are particularly interested in how the spinodal decomposition of an expanded system may lead to its multifragmentation, we demand that the most rapidly growing unstable modes be well reproduced, for each density and temperature within the spinodal zone where exponential amplification of fluctuations occurs.

This approach is akin to the simplest description of the Brownian motion in which the dynamics of pollen particles immersed in a molecular heat bath is described by a simple random force, whereas the BL approach would correspond to actually simulating the individual collisions with the gas. The method has the distinct advantage that it can be readily implemented into existing

simulation codes, in particular those employing the test-particle method, without greatly increasing the associated computational effort. We note that a more formal study of stochastic mean-field dynamics has been made previously for a very specific case [11].

The object of study is the reduced one-body phase-space density $f(\mathbf{s}, t)$ where we use $\mathbf{s} \equiv (\mathbf{r}, \mathbf{p})$ to denote a point in phase space. Presently, the most advanced dynamical model considers three distinct sources for the evolution of $f(\mathbf{s})$,

$$\frac{\partial f}{\partial t} = \{h[f], f\} + \bar{I}[f] + \delta I[f]. \quad (1)$$

The first term is the collisionless propagation of f in the self-consistent one-body field described by the effective Hamiltonian $h(\mathbf{s}) = \mathbf{p}^2/2m + U(\mathbf{r})$; this part is often referred to as the Vlasov propagation and is the semiclassical analog of the time-dependent Hartree-Fock approximation. The second source of evolution $\bar{I}[f]$ represents the average effect of the residual Pauli-suppressed two-body collisions; this is the term included in the standard BUU description. The third term $\delta I[f]$ is the Langevin term, ordinarily assumed to be Markovian and to represent the fluctuating part of the two-body collisions. The terms \bar{I} and δI can be calculated consistently by noting that the expected number of elementary transitions between the two initial and two final phase-space elements is given by [4,5]

$$d\nu_{12;34} = f_1 f_2 \bar{f}_3 \bar{f}_4 \delta(\mathbf{r}_{12}) \delta(\mathbf{r}_{34}) \delta(\mathbf{r}_{13}) \times w(p_1, p_2; p_3, p_4) d\mathbf{s}_1 d\mathbf{s}_2 d\mathbf{s}_3 d\mathbf{s}_4, \quad (2)$$

where $f_i \equiv f(\mathbf{s}_i)$ is the occupancy of the initial state i , and $\bar{f}_i \equiv 1 - f(\mathbf{s}_i)$ is the availability of the final state i . The transition rate $w(p_1, p_2; p_3, p_4)$ is related to the differential scattering cross section $d\sigma_{NN}/d\Omega$.

A convenient framework for discussing the BL problem was developed within the Fokker-Planck approximation [4,5]. The key quantities characterizing the dynamical problem are then the transport coefficients,

$$V(\mathbf{s}_i) = \langle I[f](\mathbf{s}_i) \rangle = \bar{I}[f](\mathbf{s}_i) = \frac{1}{2} \int d\nu_{12;34} (\delta_{i3} - \delta_{i1}), \quad (3)$$

$$2D(\mathbf{s}_i; \mathbf{s}_j) \delta(t_{12}) = \langle \delta I[f](\mathbf{s}_1, t_1) \delta I[f](\mathbf{s}_2, t_2) \rangle, \quad (4)$$

where the average $\langle \cdot \rangle$ is with respect to an ensemble of systems prepared with the same initial one-body density $f(\mathbf{s})$. Thus the drift coefficient $V(\mathbf{s})$ describes the average effect of the collision term. The diffusion coefficient governs the early growth rate of the correlated fluctuations in the occupancy and can be expressed explicitly as

$$D(\mathbf{s}_i; \mathbf{s}_j) = \frac{1}{4} \int d\nu_{12;34} [\delta_{ij} (\delta_{j2} + \delta_{j4}) + \delta_{i1} (\delta_{j2} - 2\delta_{j4}) + \delta_{i3} (\delta_{j4} - 2\delta_{j2})], \quad (5)$$

where $\delta_{ij} \equiv \delta(\mathbf{s}_i - \mathbf{s}_j)$, and so we may write $D(\mathbf{s}_i; \mathbf{s}_j) = D(\mathbf{p}_i, \mathbf{p}_j) \delta(\mathbf{r}_{ij})$.

The basic idea of our proposed method is to replace the actual stochastic collision term δI by a suitable stochastic one-body potential $\delta U(\mathbf{r}, t)$. The corresponding equation of motion is then obtained by making the following replacement in (1),

$$\delta I[f] \rightarrow \delta \tilde{I}[f] = -\delta F[f] \cdot \frac{\partial f}{\partial \mathbf{p}}, \quad (6)$$

where $\delta F(\mathbf{r}, t) \equiv \partial U / \partial \mathbf{r}$ is the associated Brownian force (having $\langle \delta F \rangle = 0$). Since we wish the resulting Brownian one-body dynamics to mimic the BL evolution, the stochastic force is assumed to be local in space and time. Moreover, since we wish to match its effects in nuclear matter, which is isotropic, the force may also be taken to have rotational invariance. Its correlation function can then be written

$$\langle \delta F(\mathbf{r}_1, t_1) \delta F(\mathbf{r}_2, t_2) \rangle = 2\tilde{D}_0 \mathbf{I} \delta(\mathbf{r}_{12}) \delta(t_{12}), \quad (7)$$

where \mathbf{I} is the unit tensor. The resulting dynamics is then qualitatively similar to that resulting from the BL equation (1) but the associated diffusion coefficient is modified,

$$2\tilde{D}(\mathbf{s}_1; \mathbf{s}_2) = 2\tilde{D}_0 \frac{\partial f(\mathbf{s}_1)}{\partial \mathbf{p}_1} \cdot \frac{\partial f(\mathbf{s}_2)}{\partial \mathbf{p}_2} \delta(\mathbf{r}_{12}). \quad (8)$$

The momentum dependence of the modified diffusion coefficient (8) differs from that associated with the original Boltzmann-Langevin term (5). Consequently, the replacement (6) cannot correctly mimic the entire dynamics. However, it may be possible to adjust the strength parameter \tilde{D}_0 so that those modes that dominate the evolution are well reproduced. One would expect that the unstable modes are the most essential, since they may lead to catastrophic transformations of the system. We therefore seek to reproduce the fastest growing modes inside the spinodal instability region.

In order to establish a formal basis for making such a replacement, we first recall the properties of unstable nuclear matter. The agitation of collective modes in nuclear matter inside the spinodal zone was recently addressed within the framework of linear-response theory [9]. Starting from a spatially uniform phase-space density of Fermi-Dirac form $f^0(\epsilon)$ the dynamics of small deviations $\delta f(\mathbf{r}, \mathbf{p}, t) = f(\mathbf{r}, \mathbf{p}, t) - f^0(\epsilon)$ was considered. The corresponding linearized BL equation is given by

$$\frac{\partial}{\partial t} \delta f + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \delta f - \frac{\partial U}{\partial \rho} \frac{\partial f^0}{\partial \epsilon} \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \delta \rho = \bar{I} + \delta I, \quad (9)$$

where the left-hand side describes the collisionless (Vlasov) propagation. The effect of the average collision term \bar{I} is relatively small [12,13] and is therefore ignored in the present exposition. The unstable Vlasov eigenmodes are plane waves of the form $f_{\mathbf{k}}^{\nu}(\mathbf{p}) \exp(i\mathbf{k} \cdot \mathbf{r} + \nu t/t_k)$ with $\nu = \pm$ and

$$f_{\mathbf{k}}^{\nu}(\mathbf{p}) = \frac{\partial U_{\mathbf{k}}}{\partial \rho} \frac{\mathbf{k} \cdot \mathbf{p}}{\mathbf{k} \cdot \mathbf{p} + i\nu m/t_k} \frac{\partial f^0}{\partial \epsilon}. \quad (10)$$

Here the Fourier component $\partial U_k / \partial \rho$ is simply related to the corresponding Landau parameter $F_0(k)$ [9,13,14]. The characteristic time t_k is determined by the associated dispersion relation, $h^{-D} \int d\mathbf{p} f_k^v(\mathbf{p}) = 1$.

The analysis can be further simplified by the introduction of the associated dual basis functions [15],

$$\hat{f}_k^v(\mathbf{p}) = \frac{i\nu \mathcal{N}_k}{\mathbf{k} \cdot \mathbf{p} + i\nu m/t_k}, \quad (11)$$

which have the convenient property $h^{-D} \int d\mathbf{p} \hat{f}_k^v(\mathbf{p})^* \times f_{k'}^{v'}(\mathbf{p}) = \delta_{\nu\nu'}$.

The source terms $\mathcal{D}_k^{\nu\nu'}$ governing the agitation rates of the unstable modes can then be obtained by a simple projection of the BL diffusion coefficient [15],

$$\mathcal{D}_k^{\nu\nu'} = \int \frac{d\mathbf{p}_1}{h^D} \frac{d\mathbf{p}_2}{h^D} \hat{f}_k^v(\mathbf{p}_1)^* D(\mathbf{p}_1, \mathbf{p}_2) \hat{f}_k^{v'}(\mathbf{p}_2). \quad (12)$$

This expression can be directly estimated numerically [9,14] or analytically [13,16], taking advantage of the dispersion relation and of the low-temperature approximation for the diffusion coefficient [10].

Turning now to the Brownian one-body dynamics, we can obtain the corresponding collective source terms by replacing D by \tilde{D} in Eq. (12). Exploiting the dispersion relation, we then find

$$\tilde{\mathcal{D}}_k^{\nu\nu'} = \nu\nu' \tilde{D}_0 \frac{\mathcal{N}_k^2}{m^2 k^2} \left(\frac{\partial U_k}{\partial \rho} \right)^{-2}. \quad (13)$$

We now demand that the BL results for the fastest growing mode, for any given density and temperature, be well reproduced by the Brownian one-body dynamics, i.e., we impose the matching condition $\tilde{\mathcal{D}}_k^{++} = \mathcal{D}_k^{++}(\rho, T)$, where k is the wave number associated with the shortest growth time t_k in nuclear matter having been prepared with density and temperature characteristic of the conditions prevailing in the neighborhood of the specified position \mathbf{r} . The determination of the local density $\rho(\mathbf{r})$ is relatively straightforward in the test-particle method, whereas the local equivalent temperature is somewhat more problematic. We prefer to determine $T(\mathbf{r})$ by exploiting the simple relationship between the temperature and the collision rate which is automatically available in the BUU treatment; this method does not require the momentum distribution to be thermalized. It should be noted that the Brownian force is only employed when the local conditions are inside the spinodal region of the phase diagram.

In this manner the strength can be determined at each point in space $\tilde{D}_0(\mathbf{r})$ in the course of the dynamical evolution. In practice, once the local strength $\tilde{D}_0(\mathbf{r})$ has been calculated, the test particles in the neighborhood will feel the mean-field force augmented by a small amount δF_n picked from a normal distribution with a variance in each direction given by $\sigma_F^2 = 2\tilde{D}_0/\Delta t \Delta V$, where Δt and ΔV are the time and the volume over which the same force is applied. The small diffusive violation of energy and momentum conservation can easily be eliminated by a suitable correction of the effect on δF_n on the individual test particles [16].

In order to illustrate the proposed method, we consider idealized unstable matter in two spatial dimensions, using the simple Skyrme model employed earlier [8,17]. We prepare the system at half its saturation density and with a temperature of $T = 3$ MeV, which is in the region of largest instability. The fastest mode has the wave number $k \approx 0.6 \text{ fm}^{-1}$ and the points in Fig. 1 show the evolution of the associated variance σ_k , based on a sample of 25 individual dynamical simulations, each one employing $\mathcal{N} = 1500$ test particles per nucleon. The strength of the random force is $D_0 = 144 \text{ MeV}^2 \text{ fm}/c$, the value obtained by the procedure described above. The expected BL evolution (solid curve), as obtained by the analytical linear-response result taking into account the actual growth time t_k obtained in the test-particle simulation, is shown for reference. We note that the Brownian one-body evolution converges well towards the BL curve. To be more quantitative, we have also compared the numerical results with the linear-response prediction for the Brownian one-body dynamics, using the same actual growth time t_k [16]. It is clear that this analytical prediction describes the results from the numerical simulation. Moreover, the evolutions of neighboring modes are also rather similar [16], and so the proposed method does indeed imitate the corresponding BL dynamics fairly well.

We have presented a novel simulation model for nuclear dynamics in the intermediate-energy regime where the semiclassical one-body description is expected to be applicable. The method consists of augmenting the standard

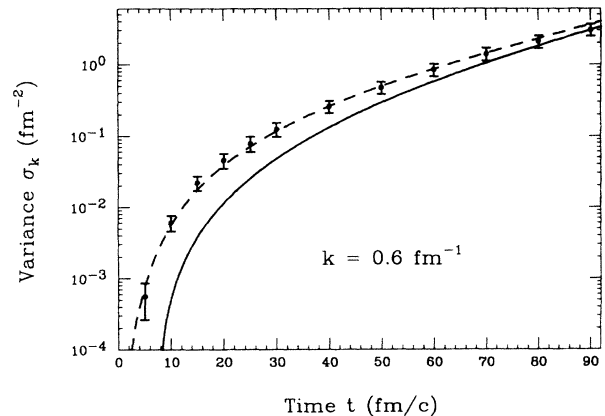


FIG. 1. Test of the method. The proposed simulation method is tested by considering the evolution of the variance σ_k of the most unstable mode in two-dimensional nuclear matter, prepared at half the saturation density and with $T = 3$ MeV. Solid curve: the expected BL result taking into account the actual growth time obtained in test-particle propagation. Points: the actual result of the Brownian one-body dynamics, with the bars representing the statistical error arising from the finite number of events. The contribution coming from the remaining small noise due to the finite number of test particle (about 5%) has been subtracted using an ensemble of events with no Brownian force. Dashed curve: the result of the corresponding linearized Brownian one-body dynamics.

BUU equation by a stochastic addition to the one-body potential $\delta U(\mathbf{r}, t)$. In the present first development along this line, the associated Brownian force $\delta \mathbf{F}(\mathbf{r}, t) = \partial U / \partial \mathbf{r}$ acts only whenever the local density and excitation corresponds to a phase point inside the region of spinodal instability, and it is then tuned so as to imitate the spontaneous agitation of the corresponding most unstable collective mode, as given by the Boltzmann-Langevin theory. This local tuning can be easily accomplished by means of simple analytical expressions for the strength parameter \tilde{D}_0 . The method can thus be implemented relatively easily into existing transport codes, especially those employing the test-particle method, and the additional computational effort is relatively modest. The resulting dynamics thus extends the standard BUU description by allowing the system to undergo bifurcations whenever the local conditions are unstable, so catastrophic processes can be addressed.

We also note that the presented method is much preferable to a recently suggested method in which the number of test particles \mathcal{N} is adjusted so that a good reproduction is obtained for the expected most dominant instability [17]. Although that method can yield useful insight under idealized circumstances, its practical applicability suffers from two major drawbacks: the need to carefully explore the nature of the instabilities encountered ahead of time and the fact that only a single quantity can be adjusted, namely \mathcal{N} , so at most one single point of the phase-space diagram could be well reproduced. Both of these drawbacks are eliminated in the present method.

In developing this method we have been motivated by the urgent need for dynamical calculations of reactions under current investigation with advanced detector arrays around the world. While the BL model is probably the presently best-founded model for this task, it is rather computer demanding in realistic scenarios. The present method offers a relatively easy tool for obtaining approximate results while more elaborate implementations are in progress and applications are presently in progress for three-dimensional multifragmentation processes [16].

We finally wish to point out that the presented approach provides a general framework for studying the kinetics of gases subject to Brownian motion and may therefore be of wider interest.

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- [1] G.F. Bertsch and S. Das Gupta, *Phys. Rep.* **160**, 190 (1988).
 - [2] W. Cassing, V. Metag, U. Mosel, and K. Niita, *Phys. Rep.* **188**, 363 (1990).
 - [3] S. Ayik and C. Gregoire, *Phys. Lett.* **B212**, 269 (1988); *Nucl. Phys.* **A513**, 187 (1990).
 - [4] J. Randrup and B. Remaud, *Nucl. Phys.* **A514**, 339 (1990).
 - [5] Ph. Chomaz, G.F. Burgio, and J. Randrup, *Phys. Lett.* **B254**, 340 (1991); G.F. Burgio, Ph. Chomaz, and J. Randrup, *Nucl. Phys.* **A529**, 157 (1991).
 - [6] F. Chapelle, G.F. Burgio, Ph. Chomaz, and J. Randrup, *Nucl. Phys.* **A540**, 227 (1992).
 - [7] G.F. Burgio, B. Benhassine, B. Remaud, and F. Seville, *Nucl. Phys.* **A567**, 626 (1994).
 - [8] G.F. Burgio, Ph. Chomaz, and J. Randrup, *Phys. Rev. Lett.* **69**, 885 (1992).
 - [9] M. Colonna, Ph. Chomaz, and J. Randrup, *Nucl. Phys.* **A567**, 637 (1994).
 - [10] J. Randrup and S. Ayik, *Nucl. Phys.* **A572**, 489 (1994).
 - [11] R. Balian and M. V  roni, *Ann. Phys.* **135**, 270 (1981).
 - [12] H. Heiselberg, C.J. Pethick, and D.G. Ravenhall, *Ann. Phys.* **223**, 37 (1993).
 - [13] J. Randrup, Report No. LBL-35848 (to be published).
 - [14] Ph. Chomaz and M. Colonna, *Phys. Rev. C* **49**, 1908 (1994).
 - [15] S. Ayik, Ph. Chomaz, M. Colonna, and J. Randrup, Report No. LBL-35987 (to be published).
 - [16] A. Guarnera, Ph. Chomaz, M. Colonna, and J. Randrup (to be published).
 - [17] M. Colonna, G.F. Burgio, Ph. Chomaz, M. Di Toro, and J. Randrup, *Phys. Rev. C* **47**, 1395 (1993).